

# **The Combined Hazard Index Calculated from Release Rate Data**

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## EXECUTIVE SUMMARY

The Ohio State University (OSU) Rate of Heat Release Calorimeter has been modified to measure selected toxic gases in the combustion products from an aircraft material test specimen. Through application of simple fire and survival models, an index for rating the fire hazard of a material tested in the OSU Calorimeter has been proposed based on the heat and toxic gases measurements taken (Combined Hazard Index, or CHI). This technical note presents the theory and documents the software used to calculate a CHI using OSU Calorimeter data.

## INTRODUCTION

### BACKGROUND.

The determination of the level of fire hazard within a burning aircraft is an immensely complicated task. Because of uncertainty of predicting full-scale phenomena from laboratory tests, full-scale tests must be run. These tests are, however, extremely expensive in terms of materials and time. Once conducted, the relative importance of factors such as temperature, smoke, and toxic gases must be evaluated, and the importance of each contributing aircraft component that should be changed or restricted must be determined. Clearly, a mathematical model of the fire event, based on small-scale material burns is desirable. Should such a model be verified, the cost savings for evaluation of a new untested material, as though part of the configured aircraft, would be immense. The complexity of such a model, however, is equally immense. As a fire progresses, many materials are exposed to varying heat flux levels, which in turn effect the subsequent progression of fire hazards.

A first step has been taken in the form of the Combined Hazard Index methodology developed by McDonnell-Douglas under Federal Aviation Administration (FAA) contract and presently used at the FAA Technical Center. The test method at the heart of the model is the Ohio State University Rate of Heat Release Calorimeter currently under consideration by American Society for Testing and Materials (ASTM) as a standard test method (reference 1). In addition to the standard parameters of heat and smoke release, gas release rates are also measured. Carbon monoxide, hydrogen cyanide, carbon dioxide, oxygen, hydrocarbons, and nitrogen oxides release rates as well as heat and smoke, are measured continuously via computer. Discrete batch samples are taken for hydrogen chloride, fluoride, and bromide. Since the Ohio State University (OSU) is a flow-through system, the rate of gas production is measured with the integral of this rate curve as the total amount of heat, smoke, or gas versus time.

A simple model to predict full-scale behavior is to burn a single material at a single heat flux, assume a fixed area that material is burning in a fixed volume container (test article). By adding the toxic gas dosage effects with the thermal toxicity (heat only incapacitation), prediction of survivability time is possible. This is the Combined Hazard Index. A more complicated task is then to use this data to describe the effects of fire propagation, heat transfer, and linear combinations of materials and heat fluxes to begin to predict full-scale fire behavior.

### THEORY.

The Combined Hazard Index is a method by which escape time from within an enclosure containing pyrolysis products is predicted mathematically. The major assumption made is that the toxic effects of individual gases and temperature are additive. For example, a concentration  $C_1$ , of a toxic gas is known to produce incapacitation at a given time,  $t_i$ . At half the concentration  $0.5 C_1$ , the test subject is half incapacitated at that same time,  $t_i$ . The Fractional Effective Dose (FED) is 1 in the first instance and 0.5 in the second. Another concentration of a second gas,  $C_2$ , is also known to produce incapacitation at the same time,  $t_i$ . If a subject is exposed to a mixture of gases 1 and 2 at the concentrations,  $1/2C_1 + 1/2C_2$ , the additivity assumption is that the subject will also incapacitate the  $t_i$ .

Inherent in this assumption is that there is no synergism or antagonism (effects which would make a mixture more or less toxic than the individual combined effects) and that there are no changes in the respiratory volume of the test subject.

Mathematically, this is expressed by Haber's Law (reference 2) which states

$$C \times T = K \quad \begin{array}{l} C = \text{Concentration} \\ T = \text{Time} \\ K = \text{Constant} \end{array} \quad (1)$$

or by rearranging

$$1 = \frac{C \ T}{K} \quad \text{where } K \text{ is expressed in units of ppm min}$$

When  $C_i$  is not a constant but a time dependent variable for gas  $i$ , incapacitation has occurred when the integral of  $C_i$  divided by  $K_i$  equals 1. For a mixture of gases where the additivity principle holds.

$$FED_i = \int_0^t \frac{C_i}{K_i} dt \quad (2)$$

$$FED = \sum_{i=1}^n FED_i = \int \frac{C_1}{K_1} dt + \int \frac{C_2}{K_2} + \dots + \int \frac{C_i}{K_i} dt \quad (3)$$

While this relationship is for gas exposures, any hyperbolic curve for toxicity may be considered, including thermal collapse. It must be kept in mind that such equations provide only for a first order approximation. Toxicity is a biological parameter and can only be measured with a biological instrument (test subject) and human toxicity can be measured only with the experimental limitation of animal models. The fractional effective dose constant,  $K$ , may be derived from  $LD_{50}$  data (Lethal Dose),  $EC_{100}$  data (Effective Concentration), or other time/response approximations. The approximation used by McDonnell-Douglas is based on occupational exposure. Extrapolation of the Threshold Limiting Value for a gas is done by multiplying the allowable concentration times the minutes in an 8-hour day.

The Combined Hazard Index will use OSU chemical data (reference 3) and make the assumption that a given amount of material is burning within a test article under uniform known heat flux conditions. The gases released by the material are instantaneously mixed throughout the test article, and there are no wall losses or further gas reactions. The heat from the material increases the air temperature and thermal collapse is a component of the FED. The test article size defines the amount of air heated, but no wall loss (absorption of heat) occurs, hence, an adiabatic boundary condition. However, there is no external source of heat increasing the test article temperature which is responsible for causing the material to burn.

The chemical components of toxicity are calculated based on the concentration accumulating in the test article from the material decomposition. Since OSU concentrations are rate data, the integral of the rate will be the test article concentration.

Where

- $\bar{C}_i^o$  = measured concentration exiting the OSU (ppm)  
 $\bar{C}_i$  = concentration predicted in the test article (ppm)  
 $A$  = sample area burned in the test article ( $m^2$ )  
 $V$  = test article volume ( $m^3$ )

OSU is run in accordance with proposed ASTM conditions i.e., 6" x 6" sample, .01 $m^3$ /sec inner pyramidal section flow rate

$$\bar{C}_i = A \frac{\int_0^t \bar{C}_i^o \times .01 \frac{m^3}{sec} \times \frac{60 sec}{min}}{36 \frac{in^2}{in} \times \frac{2.54 cm}{in}^2 \times \frac{1 m^2}{(100^2) cm^2}} \quad (4)$$

$$\begin{aligned} \bar{C}_i &= \frac{25.83 A}{V} \int_0^t \bar{C}_i^o dt \\ FED_i &= \int_0^t \frac{\bar{C}_i}{K_i} dt \\ FED_i &= \int_0^t \left( \frac{25.83 A}{V} \int_0^t \bar{C}_i^o dt \right) \frac{1}{K_i} dt \\ FED_i &= \frac{25.83 A}{V K_i} \int_0^t \int_0^t \bar{C}_i^o dt dt \end{aligned} \quad (5)$$

The Thermal component of toxicity (reference 4) for humans is based on the following relationship (reference 4)

$$t_c = \frac{4.1 \times 10^8}{T^{3.61}} \quad (6)$$

The fraction of thermal collapse,  $FED_T$ , will be an incremental time,  $dt$ , at a temperature  $T$ , divided by the time to collapse,  $t_c$ , for that temperature  $T$  ( $^{\circ}C$ ), or

$$FED_T = \int_0^t \frac{dt}{t_c} = \int_0^t \frac{T^{3.61}}{4.1 \times 10^8} dt \quad (7)$$

The temperature rise in the volume of the test article, with the constraints of the model discussed above (no wall loss, ventilation, etc.), is simply the change in air temperature of the test volume based on the heat released by the material (reference 5).

Where

T= temperature within  
the test article (C°)

Q= heat release per]  
square meter(K Watt)

Ma= mass of air  
within the test  
article (g)

Cp= heat capacity of  
air at temperature  
T (cal/gram)

V= test article volume  
(M<sup>3</sup>)

$$\frac{dT}{dt} = \frac{QA}{Ma Cp}$$

$$Ma = \frac{1.293 \times 10^3 (273.2) V}{(T + 273.2)}$$

$$Cp = .23929 + .000012T$$

$$\frac{dT}{dt} = \frac{Q \frac{1000 \text{ kW}}{\text{W}} \frac{860 \text{ cal}}{\text{Watt hr}} \frac{1 \text{ hr}}{60 \text{ min}} A}{(.23929 + .000012T) \left( \frac{1.293 \times 10^3 (273.2)}{T + 273.2} \right)} \quad (8)$$

$$T - T_0 = \int_0^t \frac{1.43 \times 10^4 A Q}{(.23929 + .000012) \left( \frac{3.50 \times 10^5}{T + 273.2} \right) V} dt \quad (9)$$

The initial temperature is 20° C. As an approximation, T is substituted for each increment dt and the equation is iteratively integrated. The temperature value is the substituted into the FED<sub>T</sub> equation and thermal collapse is predicted at that time when FED<sub>T</sub> = 1.

Q, the heat release, may be calculated via two independent methods. The Standard OSU method involves calibrating a thermopile with a known flow of methane. A known heat release rate as calculated from the methane flow is accompanied by a voltage



rise on the thermopile. Since the voltage is proportional to heat release, a simple calibration factor ( $K_H$ ) multiplied by the voltage change will correspond to a heat release rate.

$$\dot{Q}_H = \frac{(210.8 - 22.0) \text{ Kcal}}{\frac{22.4 \text{ l STP}}{\text{mole}} \left( \frac{273.2+T}{273.2} \right) \left( \frac{760}{p - \partial P_{H_2O}} \right) \left( \frac{.041433 \text{ Kcal}}{\text{K Watt min}} \right)} \quad (10)$$

Where

210.8 = Heat of combustion of methane (K cal)

22 = Heat of vaporization of  $2H_2O$  (K cal)

$$\text{Calibration factor} = K_H = \frac{\dot{Q}_H}{(E_i - E_o)}$$

Where  $E_i$  = equilibrated  
thermopile voltage

$E_o$  = initial thermopile  
voltage

$$\text{Heat Release Rate } \frac{KW}{m^2} = E_m - E_o (K_H) = E_m - E_o \frac{\dot{Q}_H}{E_i - E_o} \quad (11)$$

Where  $E_m$  = experimental  
thermopile voltage

Alternatively, heat release can be measured by oxygen depletion in the exhaust stack (reference 6). For complete combustion to  $CO_2$ ,  $16.7 \text{ MJ/M}^3 O_2$  is liberated. By having a known flow rate of air passing through the OSU, the heat release can be measured by the decrease in oxygen concentration.

$$\dot{Q} = 1.67 \times 10^4 (X_o V_a - X_s V_s) \quad (12)$$

Where

$$\dot{V}_a \approx \dot{V}_s = .01 m^3/sec$$

$X$  = Mole fraction of  $O_2$   
in air, .209

$X$  = measured fraction  $O_2$   
during the burn

$$\text{Heat Release Rate} = \frac{\dot{Q}}{A} = \frac{1.67 \times 10^4 (.01) (X_0 - X_S)}{.02323}$$

$$\frac{\dot{Q}}{A} = 7.189 \times 10^3 (X_0 - X_S) \quad (13)$$

The thrust of the Combined Hazard Index then is to define the fractional effective dose versus time by burning a material at a given heat flux and to evaluate materials on the basis of time to incapacitation as predicted by the mathematical arguments above.

Software description is shown in figure 1. Briefly, program lines 0-26 load data from a run into memory and initialize the variables, with the addition of statements 43-49 which load acid gas data if the run was supported with HF, HCl, and HBr analysis. Statements 27-42 plot the axes and label the run. Statements 50-82 plot all of the individual fractional effective doses for each gas as well as the thermal fractional effective dose. Statements 83-88 plot the total fractional effective dose. Statements 89-116 label the axes, and print the thermal and total time to incapacitation.

Automated data acquisition for CO, CO<sub>2</sub>, O<sub>2</sub>, NO<sub>x</sub>, CH<sub>x</sub>, HCN, smoke and thermopile has previously been run, with each channel sampled every 2 seconds (dt), and the data has been placed on tape. If the run was supported for acid gases, this data has been placed on a different tape file. The program described here is plotter control only; for acquisition details refer to report No. DOT/FAA/CT-TN83/1.

Statements 0-7      Display the program name, dimension the data file which will be plotted, and load the data file from tape into memory.

Statements 8-16      Print out the material burn conditions, to verify that the data is that which is desired. Also, the test article size and area of sample to be modeled by CHI is requested (Variables V and A in equations 4 and 5).

Statements 17-26      Dimension the array variables which will contain the reduced data. The S array contains the  $\frac{1}{K_i}$  toxicity constants.

T(301)= Thermopile baseline  
corrector file

Q(301)= Individual FED for temperature  
and each gas

P (301)= Combined FED

S (11) = Constants  $\frac{1}{K_i}$

Values=  $\frac{1}{480 \times \text{TLV}}$  (Threshold Limiting Value  
or the EPA concentration  
allowable for an 8-hour  
workday)

<pre> 0: fwt 1,f2.0,"/ ",fz2.0 1: fxd 0 2: dsp "CHI Plot ter control" 3: wait 5000 4: dim A[5],B[6] ,B#[20],C[11], C#[8,20],R[8, 301],T#[1] 5: ent "Input tape track and file #",A,B 6: trk A 7: ldf B,A[*], B[*],B#,C[*], C#,R[*],T# 8: wrt 16.1,A[1] ,A[2] 9: prt B# 10: spc 11: prt "Materia l #",B[1] 12: prt "Burn", B[2] 13: fxd 1 14: prt "W/cm<sup>2</sup>" ,B[3] 15: enp "Test Article Vol",C 16: enp "Materia l Area",D 17: dim S[11]; 25.83*D/C+S;1/ 24000+S[1];1/ 750000+S[2]; 1+S[3];1+S[4] 18: 1/2400+S[5]; 1/480+S[6];1+S[ 7];1+S[8] 19: 1/1440+S[9]; 1/2400+S[10];1/ 1440+S[11] 20: dim T[301]; K[8],Q[301], P[301],A#[1] 21: 3+K[1];1+K[2] ;6+K[3];5+K[4] ;2+K[5];9+K[6]; 10+K[7];11+K[8] </pre>	<pre> 22: trk 1 23: if B[3]=2.5; ldf 0,T[*] 24: if B[3]=5; ldf 1,T[*] 25: if B[3]=7.5; ldf 2,T[*] 26: 2+A;20+E 27: fxd 0 28: scl -50,650, -.1A,1.05A 29: axe 0,0,30, .05A 30: plt 180,A,1 31: csiz 3,2 32: lbl B#,B[1] 33: 8+len(B#)+B 34: cplt -B,-.8 35: csiz 2,2 36: lbl "Burn", B[2],",", 37: fxd 1 38: lbl B[3]," W/cm<sup>2</sup>" 39: if T#="p"; lbl ", piloted" 40: if T#="n"; lbl ", non- piloted" 41: cplt -35,-1 42: fxd 2;lbl D, " m<sup>2</sup> material in "ifxd 0;lbl C," m<sup>3</sup> volume" ifxd 0 43: ent "Acid Gas Analysis? (y/n)",A# 44: if A#="y"; 8+F;dsp "Insert Acid Gas Tape; press cont."; stp 45: if A#="y"; dim E[3],E#[20] ,F#[1],G[3,20], G#[3,3] </pre>	<pre> 46: if A#="y"; ent "Enter Trac k#, File#",G,H; trk G;ldf H,E[*] ,E#,F#,G[*],G# 47: if A#="n"; 5+F;eto 50 48: for J=1 to 3;if B[J]#E[J] or T##F#;dsp "WRONG ACID DATA";wait 2000 ;eto 46 49: next J 50: for M=1 to F 51: K[M]+1 52: if I&lt;9;eto 58 53: if I&gt;8;for L=1 to 20 54: if L=1;G[I- 8,1]/15+Q;for K=1 to 15;P+ Q+P;P+Q[(L-1)* 15+K];next K; eto 57 55: if L&gt;1;(G[I- 8,L]-G[I-8,L- 1])/15+Q;for K=1 to 15;P+ Q+P;P+Q[(L-1)* 15+K] 56: next K 57: next L 58: pen 59: plt 0,0,-2 60: for J=1 to 301 61: if I&gt;8;eto 73 62: if I=3;1.67e 2+.01*(C[3]- F[3,J])/(.02323+ F[3,J]) 63: if I=3;1.43e 4*D+R[3,J]*.033 33/(.2393+1.2e- 5+E)(3.5e5/(E+ 273.3)+C)+R[3, J] </pre>
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FIGURE 1. SOFTWARE LISTING (1 of 2 Sheets)

```

64: if I=3;E+
  R[3,J]+E;E+3.61
  /4.1e8+R[3,J]
65: if I=3;R[I,
  J]/30+T+T;T+
  Q[J]+Q[J]
66: if I=8;(R[8,
  J]-C[11])*(C[10]
  *1000+R[8,J]
67: if I=8;1.43e
  4*D*R[8,J]*.033
  33/(.2393+1.2e-
  5*E)(3.5e5/(E+
  273.2)*C)+R[8,
  J]
68: if I=8;E+
  R[8,J]+E;E+3.61
  /4.1e8+R[8,J]
69: if I=8;R[I,
  J]/30+T+T;T+
  Q[J]+Q[J]
70: if I#3;if
  I<8;R[I,J]*S/
  30+T+T;T*S[I]/
  30+U;U+V+Q[J];
  U+V+V
71: if I=3;if
  Q[J]<1;J*2/60+Z
72: if I=8;if
  Q[J]<1;J*2/60+Z
73: if I>8;Q[J]*
  S/30+T+T;T*S[I]
  /30+U;U+V+Q[J];
  U+V+V
74: Q[J]+P[J]+P[
  J]
75: if Q[J]>1.5;
  if Q[J]<1.65;
  plt (J+1)*2,
  Q[J];jmp 3
76: if Q[J]>1.65
  ;jmp 3
77: plt (J+1)*2,
  Q[J]
78: next J
79: csiz 1.5,2;
  if I<9;lbl C#[I
  ]
80: if I>8;lbl
  G#[I-8]
81: 0+T;0+U;0+V;
  20+E;for N=1
  to 301;0+Q[N];
  next N
82: next M
83: for J=1 to
  301
84: if P[J]<1;J*
  2/60+Y
85: if P[J]>1.5;
  if P[J]<1.75;
  plt (J+1)*2,
  P[J];jmp 3
86: if P[J]>1.75
  ;jmp 3
87: plt (J+1)*2,
  P[J]
88: next J
89: lbl "Total"
90: csiz 1.5,2
91: for K=1 to
  10
92: plt 60*K-20,
  -.05A,1
93: lbl K*60
94: next K
95: pen;plt 240,
  -.1A,-2
96: csiz 2,2
97: lbl "Time
  (sec)"
98: plt -30,.3A,
  -1
99: csiz 2,2,8/
  11,90
100: lbl "Fracti
  onal Effective
  Dose"
101: csiz 1.5,2,
  8/11,90
102: for L=1 to
  10
103: plt -10,
  .1A*L-.035*A,1
104: fxd 1
105: lbl A*.1*L
106: next L
107: csiz 2,2,8/
  11,0
108: plt 380,
  .6A,1
109: lbl "Time
  to Incapacitati
  on"
110: plt 380,
  .55A,1
111: csiz 1.5,2;
  fxd 1
112: fxd 2;lbl
  "Thermal - ",Z,
  " minutes"
113: plt 380,
  .5A,1
114: lbl "Total
  - ",Y," minut
  es"
115: plt 600,A,-
  1
116: end
*18087

```

FIGURE 1. SOFTWARE LISTING (2 of 2 Sheets)

S(1) = Carbon Monoxide  
S(2) = Carbon Dioxide  
S(8) = Oxygen (not plotted)  
S(4) = Hydrocarbons (not plotted)  
S(5) = Nitrogen oxides  
S(6) = Hydrogen cyanide  
S(7) = Smoke (not plotted)  
S(8) = Thermopile (not plotted)  
S(9) = Hydrogen Fluoride  
S(10) = Hydrogen Chloride  
S(11) = Hydrogen Bromide

S(3,7,8) = 1, they are not used for gas incapacitation, but are included to keep the data structure simplified and consistent with the acquisition channels.

K(8) = selects the channel being plotted in the FED and allows 3,7, and 8 to be ignored.

A = 2, the axis (FED) full-scale range

E = 20, the initial temperature of the test article.

Statements 27-42 Plot and establish the range of the axes and label the graph as to material, burn number, heat flux, etc. Statements 28 and 29 draw the axis. Statements 30, 34 and 41 position the labeling. The run identity (B variables) have been obtained from the tape file loaded into memory and defines the OSU burn unambiguously.

Statements 43-49 Load the acid gas file on tape into memory, if acid gas analysis accompanied the run. Statement 45 allocates memory space, 46 requests the tape location and loads it. Statements 48 and 49 check to see that the acid gas file corresponds to the same OSU burn as the previous data. The variable F corresponds to the number of individual FED curves which make up the total FED.

Statements 50-82 Controls the plotting of each FED. Statement 51 assigns the acquisition channel as the variable to be plotted.

Statements 54-57 Fill the acid gas files with interpolated values. Since 20 acid gas samples are drawn, one every 30 seconds, linear interpolation is needed to fill values between each sample to make the calculations consistent with the 2 sec dt value used to solve equation 5. This is done by subtracting the concentration of sample I from I+1 and dividing by 15. That increment is then added to sample I fifteen times, loading each value into the array which will be processed and plotted in statements 60-78. Two statements are needed to do this, one for the first sample which always has zero as its predecessor and one for the other 19 samples.

Statement 60        Creates the loop which processes each of the 301 points of acquisition data for each channel. The loop is terminated at statement 78.

Statements 62-65    Calculate the  $FED_T$  values for thermal incapacitation based on equation 13, heat release calculated from oxygen depletion. Statement 62 is the heat released. Statement 63 is the test article temperature. Statement 64 is the FED increment with Statement 65 the FED at the time of the last incremented change, based on equation 7.

Statements 66-69    Calculates the  $FED_T$  values based on heat release, calculated from thermopile voltages as in equation 11. Structure is identical to the arguments above.

Statement 70        Calculates the FED values for CO, CO<sub>2</sub>, NO<sub>2</sub> and HCN based on equation 5.

Statements 71-72    Save the value for thermal incapacitation. ( $FED = 1$ ,) while the plotting program continues.

Statement 73        Calculates the FED values for HF, HCl, HBr based on equation 5.

Statement 74        Adds the latest calculated FED value, one point at a time, to all previous FED values. This, then, is the total FED in equation 3.

Statement 75-76    Control the plotter so that FED curves do not proceed through the title of the graph. This causes exit from the loop before 10 minutes if the FED exceeds 1.65.

Statements 77        Plots all of the individual FED curves for temperature and toxic gas.

Statement 78        Ends the loop for plotting the current acquisition channel.

Statement 79-81    Print the name of the FED curve just plotted and initialize the Q array for the next FED curve.

Statement 82        Advances to the next FED curve by returning to statement 50.

Statement 83-89    Plots the total FED file which was created in statement 74. Statement 84 saves the time at which  $FED = 1$ . Statements 85 and 86 terminates the plot before it draws on the title, while Statement 87 does the plot of the curve itself and Statement 89 labels the curve.

Statements 90-97    Label the x-axis (time in 30-second increments). Statement 92 positions the numbering that is executed in statement 93.

Statements 98-106   Label the y-axis (Fractional Effective Dose). Statement 98 locates the label. Statements 102-106 number the axis with statement 103 locating the position of the numbers.

Statements 107-114 Identify the time value for thermal incapacitation and total methodology. Statements 108, 110, 114 place the labels on the graph and statements 112 and 114 write the times of incapacitation predicted to occur with the test article for the material burn in question.

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